Overview – Chemical and Scoring Ranking Assessment Model

SCRAM: A Scoring and Ranking System for Persistent, Bioaccumulative, and Toxic Substances for the North American Great Lakes *

Part I: Structure of the Scoring and Ranking System *(ESPR No. 1, 2000)* **DOI: http://dx.doi.org/10.1065/espr199910.009**
Part II: Bioaccumulation Potential and Persistence *(ESPR No. 2, 2000)* **DOI: http://dx.doi.org/10.1065/espr199910.010**
Part III: Acute and Subchronic or Chronic Toxicity *(ESPR No. 3, 2000)* **DOI: http://dx.doi.org/10.1065/espr199910.011**
Part IV: Results from Representative Chemicals, Sensitivity Analysis, and Discriminatory Power *(ESPR No. 4, 2000)* **DOI: http://dx.doi.org/10.1065/espr199910.012**

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Part I: Structure of the Scoring and Ranking System

Hundreds of chemical contaminants have been identified in the Great Lakes System of North America. Depending on the agency or organization, various subset lists of these contaminants have been identified as chemicals of potential concern. However, there is no agreement on the method that should be used to make management decisions. Except for consensus on approximately 40 chemicals that most North American agencies agree can cause deleterious effects if released into the environment, no agreement has been reached regarding the priority that contaminants should receive for further action. That leaves hundreds of chemicals that have been, are being, or potentially could be released into the environment that have not been evaluated yet. A profile for potential chemicals of concern is generally thought to include persistence in the environment, potential to bioaccumulate, and ability to cause toxic effects at environmentally relevant concentrations. Except for the International Joint Commission's definition of persistence (> 8 weeks residence time in air, water, soil or sediment), there is little concurrence about what defines these characteristics. For instance, the State of Michigan currently has no established definitions or profiles of persistent, bioaccumulative, toxic substances. Furthermore, there is no standard process to rank chemicals relative to these characteristics. The Chemical Scoring and Ranking Assessment Model (SCRAM) has been developed to provide a process to rank-order chemicals based on these characteristics. The SCRAM system was developed primarily for use in the Great Lakes region of North America and particularly in Michigan, but it is not site-specific. Use of this system may assist in pollution prevention activities and other future chemical control efforts, allowing attention to be focused first on those chemicals likely to present the greatest hazard.

Part II: Bioaccumulation Potential and Persistence

Part I of this series introduced SCRAM, a chemical scoring and ranking system for contaminants of the North American Great Lakes. Here, in **Part II**, scoring of the bioaccumulation potential and persistence of chemicals is discussed, including acceptable types of data, specific scoring instructions, and the basis for criteria and scores for these categories of the system. Difficulties encountered during the process of determining which types of data adequately represent the properties of interest are discussed. Also, justification is given for an emphasis on scoring on the basis of persistence.

Part III: Acute and Subchronic or Chronic Toxicity

In **Part II**, scoring of the potential for a chemical to persist in the environment and bioaccumulate was described. In **Part III**, scoring of chemical toxicity is discussed, including definitions and descriptions of effects that are scored, specific scoring instructions, the basis for the criteria and scores, and specific conditions or concerns regarding the types of data used for scoring. A score for each chemical screened is determined from available test data from acute or subchronic and chronic toxicity tests conducted on aquatic and terrestrial organisms. Subchronic and chronic human health effects, including carcinogenicity, are also considered. Part IV includes an evaluation of the performance of the scoring and ranking system.

Part IV: Results from Representative Chemicals, Sensitivity Analysis, and Discriminatory Power

The Chemical Scoring and Ranking Assessment Model (SCRAM) has been described in **Parts I-III** of this series. SCRAM is a chemical scoring and ranking (CSR) system that scores chemicals on the basis of bioaccumulation potential, environmental persistence, and toxicity. **Part IV** describes various tests and descriptions of the performance of this system. A group of 21 representative chemicals was chosen and scored to test the system. For those chemicals, the percentages of the scores associated with fate-related properties and associated with data uncertainty were determined. The scoring of four of these chemicals is described in greater detail, and the suitability of the scores is discussed. An analysis of the sensitivity of the system to incomplete data sets is presented. And finally, the discriminatory power of the system is described.

* The scoring and ranking system in the form of a Lotus 123[97] spreadsheet and a description of its use are available on the Internet at http://www.epa.gov/toxteam/pbtrept/

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Part IV. Results from Representative Chemicals, Sensitivity Analysis, and Discriminatory Power

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Abstract. The Chemical Scoring and Ranking Assessment Model (SCRAM) has been described in Parts I-III of this series (Snyder et al., 1999a; 1999b; 1999c). SCRAM is a chemical scoring and ranking (CSR) system that scores chemicals on the basis of bioaccumulation potential, environmental persistence, and toxicity. Part IV describes various tests and descriptions of the performance of this system. A group of 21 representative chemicals was chosen and scored to test the system. For those chemicals, the percentages of the scores associated with fate-related properties and associated with data uncertainty were determined. The scoring of four of these chemicals is described in greater detail, and the suitability of the scores is discussed. An analysis of the sensitivity of the system to incomplete data sets is presented. And finally, the discriminatory power of the system is described.

Keywords: Acute toxicity; bioaccumulation; chemical scoring and ranking; chronic toxicity; hazard; North American Great Lakes; persistence; priority pollutants; SCRAM (Chemical Scoring and Ranking Assessment Model); uncertainty; water pollution

1 Introduction

The Chemical Scoring and Ranking Assessment Model (SCRAM) has been described in Parts **I-III** of this series (Snyder et al., 1999a; 1999b; 1999c). SCRAM is a chemical scoring and ranking (CSR) system that scores chemicals on the basis of bioaccumulation potential, environmental persistence, and toxicity. Various tests of the performance of the system were conducted and are described here.

After the initial development of SCRAM, it was unclear whether many chemicals of concern would have data available for the scoring categories. A group of 21 representative chemicals was chosen to test the system. These chemicals exhibit a wide range of fate-related properties and toxic effects, and thus would be expected to produce a range of scores. Of this group, there are chemicals for which there is a large body of data of interest here, and others about which very little is known of their potential risk to the environment. In-depth literature searches were conducted for each of these chemicals, and each was scored. The percentages of their scores due to fate-related properties and due to data uncertainty were determined. The scoring of four of these chemicals is described in greater detail, and the suitability of the scores is discussed. An analysis of the sensitivity of the system to incomplete data sets is presented. And finally, the power of the system to discriminate among chemicals with different properties is described.

A list of the ranked final scores for 21 representative test chemicals and the percentage of their final composite scores associated with uncertainty and associated with bioaccumulation and persistence is given in **Table 1**. The percentage of the score associated with fate was determined as described in Equation 1.

*The scoring and ranking system in the form of a Lotus 123[97] spreadsheet and a description of its use are available on the Internet at http://www.epa.gov/toxteam/pbtrept/

Equation 1:

Percentage of score associated with fate =

$$\left[\frac{(B_{chem} \times P_{chem} \times 1.5) + (B_{unc} \times P_{unc} \times 1.5)}{F_{comp}}\right] \times 100$$

B_{chem} = bioaccumulation chemical score
P_{chem} = persistence chemical score
B_{unc} = bioaccumulation uncertainty score
P_{unc} = persistence uncertainty score
F_{comp} = final composite score

In **Table 1**, the percentage of the score associated with uncertainty was calculated using Equation 2 for chemicals scored on the acute toxicity path and Equation 3 for chemicals scored on the chronic toxicity path.

Equation 2:

Percentage of score associated with uncertainty =

$$\left[\frac{(B_{unc} \times P_{unc} \times 1.5) + AA_{unc} + AT_{unc}}{F_{comp}}\right] \times 100$$

B_{unc} = bioaccumulation uncertainty score
P_{unc} = persistence uncertainty score
AA_{unc} = acute aquatic toxicity uncertainty score
AT_{unc} = acute terrestrial toxicity uncertainty score
F_{comp} = final composite score

Equation 3:

Percentage of score associated with uncertainty =

$$\left[\frac{(B_{unc} \times P_{unc} \times 1.5) + CA_{unc} + CT_{unc} + CH_{unc}}{F_{comp}}\right] \times 100$$

B_{unc} = bioaccumulation uncertainty score
P_{unc} = persistence uncertainty score
CA_{unc} = chronic aquatic toxicity uncertainty score
CT_{unc} = chronic terrestrial toxicity uncertainty score
CH_{unc} = chronic human toxicity uncertainty score
F_{comp} = final composite score

Because part of the uncertainty score is associated with fate (P_{unc} and B_{unc}), the percentage of the score associated with fate and the percentage of the score associated with uncertainty together might equal greater than 100%.

2 Selection of the Weighting Factor for Fate Scores

A weighting factor was applied to the bioaccumulation and persistence chemical and uncertainty scores in order to increase the influence of these two fate-related (exposure-related) characteristics on the final score. SCRAM places an emphasis on environmental fate (or exposure), and particularly on environmental persistence, for scoring because it is possible that a chemical currently not known to cause serious toxic effects might later be found to be toxic through a mechanism not currently known or investigated. Also, if a chemical is not present in the environment for relatively long periods of time and/or does not bioaccumulate or bioconcentrate, chronic toxicity is not likely to be an issue of concern for the chemical. The weighting factor was set at 1.5 because this value increased the percentage of the final composite score that is associated with fate properties to an average of greater than 50% (57%) for the list of 21 representative chemicals used to test this scoring system. While the selection of this weighting factor is undeniably arbitrary, it suits the purpose of emphasizing fate-related properties for scoring. The user of this scoring system might decide to adjust the weighting factor to place more or less emphasis on fate for scoring to suit the purposes of the screening.

3 Scores of Model Chemicals

The group of 21 test chemicals was used to conduct a sensitivity analysis (see Section 4) of SCRAM. After incorporation of the weighting factor of 1.5, the maximum number of uncertainty points possible if the subchronic/chronic toxicity scoring path is taken is 89 (if no data are available), and the maximum chemical score possible is 53. If the acute toxicity scoring path is taken, the maximum number of uncertainty points is 85 (if no data are available), and the maximum chemical score possible is 48. Based on the range of properties and availability of data, the 21 representative chemicals listed in **Table 1** would be expected to produce a relatively wide range of scores. SCRAM produced a range of composite scores from a high of 62 to a low of 18. Four more detailed examples of scoring from the 21 test chemicals scored with SCRAM are presented *(→ Table 2)*.

3.1 DDT (Dichlorodiphenyltrichloroethane)

The DDT complex [consisting of the *ortho* and *para* isomers of DDT, DDE (dichlorodiphenyldichloroethylene), and DDD (dichlorodiphenyldichloroethane)] is persistent and bioaccumulative, and is toxic to some groups of organisms at environmentally relevant concentrations. The DDT complex is widely distributed as an environmental contaminant and detectable in soils, sediments, water and biota throughout the world. It receives the maximum chemical score in all categories, i.e., persistence, bioaccumulation, and chronic toxicity *(→ Table 2)*. Because of the knowledge about its fate and adverse effects properties, the data uncertainty scores it receives are relatively smaller (0, 2, and 4 for bioaccumulation, persistence, and toxicity, respectively). Its final uncertainty score is 7, one of the lowest uncertainty scores assigned to the list of 21 representative chemicals. Justifiably, DDT receives one of the greatest composite scores generated by SCRAM for this list of chemicals through a combination of the maximum possible chemical score and a limited uncertainty score.

3.2 Mercury

Mercury, like DDT, is also a persistent, bioaccumulative, and toxic environmental contaminant that is detectable in most environmental matrices, especially sediment and the flesh of some species of fish. Accordingly, it would be expected to receive one of the greatest scores of the representative chemicals. When methylated in the environment, it bioaccumulates to a relatively great degree in the aquatic food chain (score of 4), yet not as greatly as DDT (score of 5). Because it is a non-radioactive element, it receives the maximum environmental persistence score of 5 *(→ Table 2)*.

Table 1: Based on the range of properties and availability of data, the 21 representative chemicals listed would be expected to produce a relatively wide range of scores. SCRAM produced a range of composite scores from a high of 62 to a low of 18. Because part of the uncertainty score is associated with fate (P_{unc} and B_{unc}), the percentage of the score associated with fate and the percentage of the score associated with uncertainty together might equal greater than 100%.

Chemical Name	Composite Score	Chemical Score	Uncertainty Score	Percentage of Score Associated with Fate[a]	Percentage of Score Associated with Uncertainty
Acrylonitrile	23	11	12	48%	52%
Benzidine	37	22	15	46%	41%
Butylbenzyylphthalate	31	18	13	55%	42%
Carbon tetrachloride	30	18	12	43%	40%
Chlordane	60	52	8	68%	13%
p,p'-DDT	60	53	7	68%	12%
1,2-Dichloroethane	28	19	9	39%	32%
Di-n-butylphthalate	34	21	13	59%	38%
Elemental mercury	52	45	7	62%	13%
Heptachlor epoxide	53	40	13	68%	25%
Hexachloroethane	44	33	11	59%	25%
Indeno (1,2,3-cd)pyrene	54	11	43	70%	80%
Isophorone	18	7	11	50%	61%
Lindane	41	38	3	61%	7%
Naphthalene	25	13	12	36%	48%
n-Nitrosodiphenylamine	33	13	20	55%	61%
Octachlorostyrene	40	13	27	58%	68%
PCBs	61	53	8	71%	13%
Phenanthrene	42	30	12	60%	29%
Toxaphene	62	53	9	69%	15%
1,1,1-Trichloroethane	24	12	12	42%	50%
AVERAGE:				**57%**	**37%**

[a] Fate refers to bioaccumulation and persistence scoring categories.

Table 2: The bioaccumulation chemical score is multiplied by the persistence chemical score, and that product is multiplied by a weighting factor of 1.5. The resulting number is added to the toxicity chemical score to yield the final chemical score. The bioaccumulation uncertainty score is multiplied by the persistence uncertainty score, and that product is multiplied by a weighting factor of 1.5. The resulting number is added to the toxicity uncertainty score to yield the final uncertainty score. The final composite score is the sum of the final chemical score and the final uncertainty score**.**

Scoring category	CHEMICAL			
	p,p'-DDT	Elemental Mercury	Indenopyrene	Benzidine
Bioaccumulation chemical score	5	4	5	2
Bioaccumulation uncertainty score	0 [a]	1	2	1
Persistence chemical score	5	5	0 [a]	4
Persistence uncertainty score	2	0 [a]	10	3
Toxicity chemical score	15	15	3	10
Toxicity uncertainty score	4	5	13	10
Final chemical score	53	45	11	22
Final uncertainty score	7	7	43	15
Final composite score	60	52	54	37

[a] SCRAM assigns a default score of 1 in place of a zero for chemical and uncertainty scores in the bioaccumulation and persistence categories to avoid canceling out other non-zero values during the mulitiplication step.

Table 3: Only the chemical scores for bioaccumulation and persistence were used in the sensitivity analysis. Uncertainty scores were not used. The weighting factor of 1.5 was not incorporated. The results illustrate that incomplete data sets can alter greatly the composite chemical scores for bioaccumulation and persistence.

Chemical Name	BIOACCUMULATION		PERSISTENCE		PRODUCTS[a]
	Greatest Score	***Least Score***	***Greatest Score***	***Least Score***	
p,p'-DDT	5	3	5	1	25, 5, 15, 3
Heptachlor epoxide	5	2	5	1	25, 5, 10, 2
Indeno (1,2,3-cd)pyrene	5	5	0	0	5, 5, 5, 5
Elemental mercury	4	4	5	5	20, 20, 20, 20
PCBs	5	5	5	3	25, 15, 25, 15
Lindane	3	1	5	1	15, 3, 5, 1
Toxaphene	5	2	5	1	25, 5, 10, 2
Octachlorostyrene	5	5	0	0	5, 5, 5, 5
Chlordane	5	2	5	1	25, 5, 10, 2
Phenanthrene	5	2	5	1	25, 5, 10, 2
n-Nitrosodiphenylamine	3	2	3	1	9, 3, 6, 2
Hexachloroethane	5	2	5	1	25, 5, 10, 2
1,2-Dichloroethane	1	1	5	1	5, 1, 5, 1
Acrylonitrile	1	1	2	1	2, 1, 2, 1
Carbon tetrachloride	2	1	5	1	10, 2, 5, 1
Naphthalene	3	1	5	1	15, 3, 5, 1
Butylbenzylphthalate	5	2	4	1	20, 5, 8, 2
1,1,1-Trichloroethane	2	1	5	1	10, 2, 5, 1
di-N-Butylphthalate	5	1	4	1	20, 5, 4, 1
Isophorone	2	1	2	1	4, 2, 2, 1
Benzidine	2	1	4	1	8, 2, 4, 1

[a] Products are listed as follows: bioaccumulation greatest score x persistence greatest score, bioaccumulation greatest score x persistence least score, bioaccumulation least score x persistence greatest score, bioaccumulation least score x persistence least score.

Adverse effects of mercury on both aquatic and terrestrial life are well documented. Of the test chemicals scored by SCRAM, mercury received one of the smallest uncertainty scores (score of 7). Although mercury receives one of the greater chemical scores, the small uncertainty score places mercury at a lesser relative ranking than heptachlor epoxide, PCBs, and indenopyrene. This is justified by the bias of SCRAM toward ranking chemicals about which little is known higher to encourage more review of their potential for adverse effects.

3.3 Benzidine

Benzidine is a chemical identified on the International Joint Commission (IJC) Working List of chemicals as one that may have a potential for release to the North American Great Lakes System (IJC, 1989). Benzidine scores a 4 for persistence, but is not very bioaccumulative, with a bioaccumulation chemical score of 2 (→ *Table 2*). Benzidine is considered to be only moderately toxic to both aquatic and terrestrial life, with a combined toxicity chemical score of 10. Due to a moderate lack of data for both aquatic and terrestrial life, the toxicity uncertainty score is 10. Benzidine would not be expected to receive a particularly great score, and, indeed, it received a moderate final composite score of 37.

3.4 Indenopyrene

Indenopyrene is the test chemical that yields the greatest uncertainty score, as it demonstrates the least information on adverse effects. The final uncertainty score is 43, whereas the final chemical score is only 11 (→ *Table 2*). The composite score of 54 ranks indenopyrene over elemental mercury. This scoring system is biased toward giving a greater rank for uncertainty to encourage further review or research into the adverse effects and environmental fate of a chemical. The rank order may be readjusted following further review, providing a chemical is shown to be less potentially hazardous than the composite score indicates. In the case of indenopyrene, much may be determined by considering its structural similarity to other polynuclear aromatic hydrocarbons (PAHs). PAHs, in general, tend to be persistent yet often are readily metabolized by fish, precluding a great bioaccumulation potential. Several members of the PAH class demonstrate relatively little toxicity, while others demonstrate substantial evidence of carcinogenic potential. Characteristics of this class of chemicals indicate a need for further consideration of the potential adverse effects. This chemical would likely escape attention in other scoring systems, which would produce a low ranking or no scoring at all due to lack of data.

4 Sensitivity Analysis

A sensitivity analysis was conducted to determine what possible scores the system might generate if only some of the data found in the literature were used for scoring *(→ Table 3)*. For example, if a user found only a few of the data in existence, greater or lesser scores than those calculated from a complete literature review might result. To test the sensitivity of the system to incomplete data sets, the extreme cases were examined by using only those literature values that generated the greatest and least scores. Bioaccumulation and persistence chemical scores only were used for the sensitivity analysis, since these two categories account for the most substantial portion of the final score. For each chemical, the greatest and least values for bioaccumulation were used to calculate a chemical score. A similar exercise was conducted for persistence. Then the following products (sensitivity analysis scores) were calculated: greatest bioaccumulation score × greatest persistence score, greatest bioaccumulation score × least persistence score, least bioaccumulation score × greatest persistence score, and least bioaccumulation score × least persistence score. This process gives an overview of the range of possible scores that might have been calculated if the data set had been less complete.

The sensitivity analysis indicated that the selection of values from the available literature can have a great effect on the resulting scores *(→ Table 3)*. For instance, in the case of the PAH phenanthrene, the sensitivity analysis score could be as great as 25 and as little as 2, depending on the values selected from the literature to score the chemical. Alternatively, there are chemicals for which the range of sensitivity analysis scores was relatively small, as was the case with isophorone, with a range of scores from 4 to 1 *(→ Table 3)*. Because SCRAM can be very sensitive to incomplete data sets, it is extremely important that thorough literature searches be conducted to locate as many suitable data points as possible for scoring. The user's confidence in the score should be tempered by professional judgement of the level of effort given to the literature search and review process.

5 Discriminatory Power

The power of this system to discriminate among individual chemicals based on their bioaccumulation potential, persistence, and toxicity is not great. Rather, the function of SCRAM is to rank chemicals for prioritization activities, e.g., to determine which should receive the most immediate attention for risk assessment and/or research. Absolute scores have little meaning; it is the relative scores that are important. The user must also remember that a score two times greater than another does not indicate twice the level of concern.

6 Conclusions and Future Outlook

SCRAM is a chemical scoring and ranking system that deals with chemical persistence in the environment and data uncertainty in a unique manner. One of the more important features of the system is its treatment of lack of data. Chemicals receive a greater score for lack of data, thereby driving the procurement of more information. With SCRAM as the overlying framework for screening and assessment, users can tailor the data selection criteria, severity and safety factors, weighting factors and other system characteristics to meet their specific program objectives. However, objectives and modifications to data selection criteria and other characteristics must be reported with the scores and ranking. Future improvements may include incorporation of data on current use and environmental loading to improve assessment of potential for exposure or addition of a means to address ecotoxicological effects like stratospheric ozone destruction. Michigan Department of Environmental Quality (MDEQ) staff recently completed an initial screening of a much larger group of chemicals. The resulting scores may be used to adjust the system for better performance.

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